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Characteristic-based numerical schemes for generalized models in chromatography.

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The equilibrium dispersive model for liquid chromatographic processes consists in a system of nonlinear convection-diffusion partial differential equations for the concentration of each injected liquid component.

There are several difficulties posed in the numerical approximation of the solution of these equations: Firstly, the fluxes depend on the concentration of the liquid (mobile) phases, but the conserved variables are the concentration of each substance, which consists of a fraction of mobile phase and a complementary fraction of stationary phase, in which the concentration of stationary phase adsorbing each injected substance is given by nonlinear relations, the *adsorption isotherms*; Secondly, when the *apparent axial dispersion coefficient* (see [4]), i.e., the diffusion coefficient, is small but non-negligible, strong gradients are inevitably developed and the numerical schemes should cope with them by being based on conservative discretizations, which require the functional inversion of the nonlinear relationship between primitive variables (the variables the fluxes depend on) and conserved variables (see [2]); Thirdly, an explicit discretization of the diffusive fluxes may impose a stability restriction on the time step that might compromise efficiency.

In [2] Langmuir isotherms are used and the latter issues are tackled through an efficient functional inversion for getting primitive variables from conserved ones and Implicit-Explicit time-discretizations (see [1]), in which the diffusion terms are treated implicitly and the convective terms explicitly.

The burden of these techniques is that the convective fluxes are obtained through a high-order reconstruction of the components of split physical fluxes through the Global Lax-Friedrichs flux-splitting. The use of this flux-splitting (or an upwind flux-splitting) in the componentwise setting often yields spurious oscillations near discontinuities (see [3]).

In this paper we extend the techniques introduced in [2] to generalized Langmuir isotherms (Tóth isotherms) and propose a characteristic-based upwind numerical flux (see [3]) that yields oscillation-free results. Some experiments are performed to show the relative efficiency gains of the proposal.

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